The two-leg t-J ladder: a spin liquid generated by Gutzwiller projection of magnetic bands

Martin Greiter

Department of Physics, Stanford University, Stanford, CA 94305, greiter@quantum.stanford.edu (SU-ITP 98/19, cond-mat/9804002, March 31, 1998)

The ground state of the two-leg Heisenberg ladder is identified as an RVB type spin liquid, which is generated by Gutzwiller projection of tight-binding bands with flux π per plaquet. Explicit trial wave functions for the magnon and hole excitations are formulated in terms of spinons and holons.

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1. Itinerant antiferromagnets confined to coupled chains, or t–J ladders, have enjoyed enormous popularity over the past few years [1–9]. They provide the simplest example of a generic spin liquid in dimensions greater than one, and the only example thereof which is presently fully amenable to numerical methods. (It is furthermore widely believed that they constitute the first step towards understanding the two-dimensional t–J model starting from one dimension, but I rather believe the two-leg ladder to be just a special case.) These models are approximately realized in $(VO)_2P_2O_7$, $SrCu_2O_3$, and $Sr_{14-x}Ca_xCu_{24}O_{41}$, and hence accessible to experiment.

The t-J Hamiltonian for the ladder is given by

$$H_{t-J} = -\sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} \sum_{\langle ij\rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

where $(t_{ij}, J_{ij}) = (t, J)$ if i and j are nearest neighbors along one of the chains, and (t_{\perp}, J_{\perp}) if they are nearest neighbors across the rungs; each pair $\langle ij \rangle$ is summed over twice and no doubly occupied sites are allowed.

One of the most striking features of the two-leg t-Jladder is the persistence of a spin gap $\Delta \approx J_{\perp}/2$ in the weak coupling limit $J_{\perp} \ll J$. (For sufficiently strong couplings $J_{\perp} > J$, the system can be described by a perturbative expansion around the strong coupling limit consisting of singlets across the rungs [10], which yields a spin gap $\Delta \approx J_{\perp} - J + \frac{1}{2}J^2/J_{\perp}$; a weak coupling expansion starting from decoupled chains, however, is not possible, as the individual spin chains are quantum critical in the sense that the tiniest perturbation can change the universality class.) In this letter, I will formulate a microscopic theory of the two-leg t-J ladder, which is universally valid at all ratios J_{\perp}/J , in terms of explicit spin liquid trial wave functions for the ground state, magnon (spinon-spinon bound state) and the hole (holon-spinon bound state) excitations.

2. The trial wave function for the ground state of the Heisenberg ladder, the $t{-}J$ ladder without any holes, is constructed as follows. Consider a tight binding ladder with flux π per plaquet, and hopping terms of magnitude \tilde{t} along the chains, and \tilde{t}_{\perp} across the rungs. In the gauge depicted in figure 1, we write the single particle Bloch states

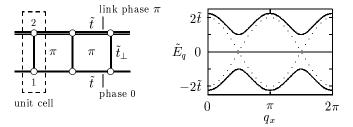


FIG. 1. Flux band structure of a tight binding ladder with flux π per plaquet for $\tilde{t}_{\perp}/\tilde{t}=0$ (doted lines) and $\tilde{t}_{\perp}/\tilde{t}=1$ (solid lines). The energy gap is given by $2\tilde{t}_{\perp}$.

$$\psi_q(j) = e^{iq \cdot R_j} u_q(j), \tag{2}$$

where the $u_q(j)$ are strictly periodic in both real and momentum space and obey

$$\tilde{H}_q \begin{pmatrix} u_q(1) \\ u_q(2) \end{pmatrix} = \tilde{E}_q \begin{pmatrix} u_q(1) \\ u_q(2) \end{pmatrix} \tag{3}$$

where

$$\tilde{H}_q = 2\tilde{t} \begin{pmatrix} \cos q_x & me^{-iq_y} \\ me^{iq_y} & -\cos q_x \end{pmatrix}$$
 (4)

with $m\equiv \tilde{t}_\perp/2\tilde{t}$. Since (3) is a two-dimensional Dirac equation, i.e. \tilde{H}_q^2 is diagonal, we immediately obtain the eigenvalues

$$\tilde{E}_q = \pm 2\tilde{t}\sqrt{\cos^2 q_x + m^2}. (5)$$

The coupling between the tight-binding chains hence induces an energy gap of magnitude $2\tilde{t}_{\perp}$. We now fill the lower band twice, once with up-spin electrons, and once with down-spin electrons; the resulting Slater determinant $|\psi_{\rm SD}\rangle$ is obviously a spin singlet. The spin liquid trial wave function for the Heisenberg ladder with $J_{\perp}/J=\tilde{t}_{\perp}/\tilde{t}$ is obtained by eliminating all the doubly occupied sites via Gutzwiller projection,

$$|\psi_{\text{trial}}\rangle = \mathcal{P}_{G}|\psi_{SD}\rangle.$$
 (6)

Since the Gutzwiller projector \mathcal{P}_{G} commutes with the total spin operator, $|\psi_{\text{trial}}\rangle$ is also a singlet. This trial wave function is as accurate an approximation as the Haldane-Shastry state [11] for the one-dimensional Heisenberg

$\overline{J_{\perp}/J}$	E_{t}	%	over-	$\left\langle ec{S}_{i}ec{S}_{j} ight angle _{\parallel }$		$\langle ec{S}_i ec{S}_j angle_{\perp}$		
	exact	trial	off	lap	exact	trial	exact	$_{\rm trial}$
0	-9.031	-9.015	0.2	0.997	-0.452	-0.451	0.000	0.000
0.1	-9.062	-9.024	0.4	0.986	-0.450	-0.451	-0.062	-0.011
0.2	-9.155	-9.073	0.9	0.969	-0.445	-0.449	-0.123	-0.045
0.5	-9.755	-9.568	1.9	0.952	-0.420	-0.413	-0.269	-0.263
1	-11.577	-11.346	2.0	0.941	-0.354	-0.302	-0.450	-0.530
2	-8.594	-8.444	1.8	0.957	-0.222	-0.143	-0.638	-0.702
5	-7.664	-7.594	0.9	0.981	-0.085	-0.029	-0.732	-0.748
10	-7.539	-7.513	0.3	0.993	-0.040	-0.007	-0.746	-0.750
∞	-7.500	-7.500	0.0	1.000	0.000	0.000	-0.750	-0.750

TABLE I. Energy expectation values and nearest neighbor spin correlations for the spin liquid trial wave functions in comparison with the exact ground states of a 2×10 Heisenberg ladder with periodic boundary conditions, as well as overlaps between trial wave functions and exact ground states. Throughout this article, all energies quoted are in units of $\max(J_{\perp},J)$. The boundary phase before Gutzwiller projection has been 0.

chain in the weak coupling limit $J_{\perp}/J = 0$, and exact in the strong coupling limit $J_{\perp}/J \to \infty$; the approximation has its worst point at isotropic coupling (see table I) [12,13].

3. There are essentially two ways of constructing spinon and holon excitations for spin liquids (they are obtained from each other by annihilating or creating an electron on the spinon or holon site). The first one is Anderson's projection technique [14]: inhomogenities in both spin and charge created before Gutzwiller projection yield inhomogenities in spin only after projection. Anderson writes a state with two spinons localized at sites i and j

$$|\psi_{i\uparrow,j\downarrow}\rangle = \mathcal{P}_{G}c_{i\uparrow}^{\dagger}c_{j\uparrow}|\psi_{SD}\rangle.$$
 (7)

In the case of the ladder, however, the spinons are not free particles, but bound into pairs by a linear confinement force [15]. To obtain the magnon trial wave function,

$$|\psi_{\text{magnon}}(k)\rangle = \sum_{i,j} \phi_{i,j}(k) |\psi_{i\uparrow,j\uparrow}\rangle,$$
 (8)

a hence nontrivial internal wave function $\phi_{i,j}(k)$ for the spinon-spinon bound state is required. (In the one-dimensional spin chain, by contrast, the spinons interact only weakly, and the internal spinon wave function can be approximated by plane waves.)

It is therefore expedient to use the second method, which has been successful in describing the fractionally charged solitons in polyacytelene [16]: Rokhsar [17] constructs elementary excitations of spin liquids via localized midgap states, which are either occupied by a single electron (spinon) or left unoccupied (holon). The topology of the ladder dictates that midgap states can only be created in pairs, which implies that we automatically obtain spinon-spinon (or holon) bound states rather then

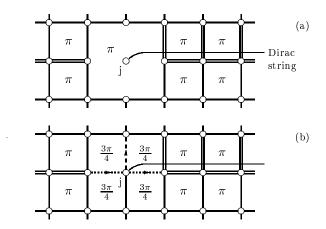


FIG. 2. Magnetic tight-binding configuration for a holon of the chiral spin liquid (a) as proposed by Rokhsar (cutting all the links to a given site and adjusting the flux according to Rokhsar's loop rules generates a stationary holon or holetto) or (b) by combining this flux adjustment with Anderson's projection technique (only the phases of the hopping parameters around the holon site are adjusted).

isolated spinons (or holons). The fact that the energy required to create two singly occupied midgap states is proportional to \tilde{t}_{\perp} suggests a spin gap proportional to J_{\perp} . These general observations, however, leave us still with a large number of possible choices for the midgap states; most constructions yield satisfactory magnon, but only very few acceptable hole trial wave functions. To identify those, let us step back and take a broader view.

4. The spin liquid proposed above is, in fact, a special case of the Kalmeyer-Laughlin chiral spin liquid [18], obtained by imposing a periodic boundary condition with a periodicity of only two lattice spacings in y-direction. This chiral spin liquid may be generated from a tight-binding lattice with flux π per plaquet and hopping magnitudes \tilde{t} and $\frac{1}{2}\tilde{t}_{\perp}$ in x- and y-direction, respectively; the P and T violating diagonal hopping elements, which are otherwise required to open an energy gap, cancel due to the boundary condition.

Spinons and holons for the chiral spin liquid may be constructed via Anderson's method or via midgap states; Rokhsar creates a midgap state in the flux band structure before projection by cutting all the links to a given site and adjusting the flux according to his loop rules, which require that the kinetic energy on the loops around each plaquet is minimal (see figure 2a). The resulting holon is not nearly as mobile as Anderson's, but optimal with regard to the magnetic energy; it adequately describes stationary charge excitations. I call it a stationary holon or holetto. To obtain the generic and mobile holon, we create a midgap state by adjusting the flux according to Rokhsar's procedure (i.e. we create a defect of flux π around the holon site) without cutting any links (i.e. we adjust the hopping phases without adjusting the magnitudes), and then project such that this site is unoccupied

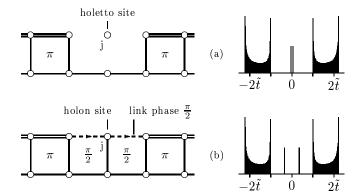


FIG. 3. Magnetic tight-binding configurations and the corresponding density of states for the ladder with a spinon bound to (a) a stationary *holetto* or (b) a mobile *holon* before Gutzwiller projection. Only the latter flux configuration violates P and T.

(see figure 2b). This holon is equivalent to Anderson's in the case of the chiral spin liquid, but more generally applicable.

5. The flux configurations used to construct holettospinon and holon-spinon bound states for the ladder are shown in figure 3a and b. In the case of the holetto, we cut all the links to a given site; as the topology of the ladder does not provide a context for a flux adjustment around this site, we obtain a second midgap state, and hence a spinon, localized nearby. This trial wave function describes a stationary hole. To construct a mobile hole, we create the midgap states by only adjusting the flux, and project such that the holon site is unoccupied; as we are creating two rather than one midgap state, we remove flux $\pi/2$ from each neighboring plaquet [19]. The flux configuration now violates P and T, and the holon-spinon bound state carries a chirality quantum number, which is + for the configuration shown in figure 3b, and - for its complex conjugate; states of opposite chiralities map into each other under P or T. The final trial wave functions for the hole is a linear superposition of the holon-spinon bound states of both chiralities at each momentum,

$$|\psi_{\text{hole}}(k)\rangle = \mathcal{N} \sum_{j} e^{ir_{j}k} \left(|\psi_{j}^{+}\rangle + a(k)|\psi_{j}^{-}\rangle \right),$$
 (9)

where r_j is the holon coordinate and a(k) is a variational parameter. Magnons or spinon-spinon bound states are obtained from the holon-spinon bound states by creating an electron at the holon site, which forms a spin triplet with the spinon bound to it.

Numerical comparisons of the trial wave functions for holes and magnons with the exact eigenstates are presented in figure 4 and in tables II–IV. The hole trial wave functions for $t_{\perp}/J_{\perp}=t/J=1$ (see table II) are excellent at stong coupling, and less accurate at isotropic coupling; for weak coupling, they are excellent only at momenta close to the one-hole ground states, as there

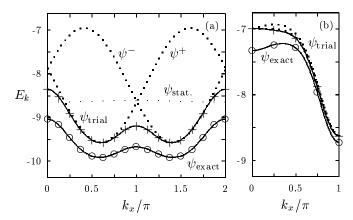


FIG. 4. Dispersions for a single (a) hole (holon-spinon bound state) and (b) magnon (spinon-spinon bound state) as predicted by the spin liquid proposed here in comparison with the exact dispersions for a 2×8 ladder with $J_{\perp}=J=t_{\perp}=t=1$ (see tables II and III) and periodic (or antiperiodic) boundary conditions. The dotted lines correspond to the individual + and – chirality trial wave functions (generated from the tight-binding configuration shown in figure 3b and its P or T conjugate, respectively) and the stationary holetto-spinon bound state (according to figure 3a), as indicated.

is a large amplitude to find a hole and a magnon rather than just a hole at other momenta. The holon-spinon bound state wave functions adequately describe the hole when t and J are comparable (see table IV); for $t \ll J$, the holetto-spinon bound state is more appropriate, while holes with sufficiently large t are detrimental to antiferromagnetic correlations and eventually destabilize the spin liquid [20]. The trial wave functions for the magnons are generally satisfactory (see table III).

6. The P and T violation of the localized holon-spinon bound states, or the appearance of a chirality quantum number, is a physical property of the system; any real trial wave function for the localized hole would yield a dispersion $E_k \propto \cos(k_x)$, and thus be inconsistent with the dispersion obtained by exact diagonalization (bottom curve in figure 4a). The chirality quantum number is a manifestation of the fractional statistics [21] of spinons and holons [18,22] in dimensions greater than one; it determines the sign of the statistical phases acquired as they encircle each other.

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J_{\perp}/J		E_{tot}		%	over-	$E_{t_{\parallel}}$		$E_{t_{\perp}}$		a
					lap					
0.2	0	-7.40	-6.88	7.1	0.560	-1.51	-0.45	0.04	0.06	1.00
	1/4	-7.92	-7.83	1.1	0.975	-1.63	-1.62	0.01	0.04	0.07
	1/2	-8.17	-8.07	1.2	0.952	-1.89	-1.87	-0.02	0.04	0.10
	3/4	-7.59	-7.22	4.9	0.540	-1.49	-1.01	-0.10	0.04	0.08
	1	-7.21	-5.98	17	0.000	-1.55	0.45	-0.09	0.06	1.00
	0				0.776					
	1/4	-9.46	-8.91	5.8	0.849	-1.21	-0.47	-0.45	-0.67	0.12
1	1/2	-9.89	-9.52	3.7	0.894	-1.54	-1.23	-0.59	-0.57	0.02
	3/4	-9.84	-9.47	3.8	0.917	-1.35	-0.99	-0.81	-0.70	0.16
	1	-9.67	-9.19	5.0	0.917	-1.07	-0.42	-0.98	-0.89	1.00
5	0	-6.20	-6.12	1.3	0.981	0.13	0.19	-0.96	-1.00	1.00
	1/4	-6.25	-6.18	1.1	0.984	0.08	0.11	-0.97	-0.99	0.32
	1/2				0.987					
	3/4				0.988					
	1	-6.55	-6.50	0.7	0.988	-0.21	-0.19	-1.00	-1.00	1.00

TABLE II. Energy expectation values including individual contributions to the kinetic energy from chains and rungs and overlaps for the trial wavefunctions describing holon-spinon bound states in comparison with the exact one hole eigenstates for a periodic 2×8 ladder with $t_{\perp}/J_{\perp}=t/J=1$ for three ratios J_{\perp}/J . The energies are in units of $\max(J_{\perp},J)$; the transverse momentum is always $k_y=0$, as a $k_y=\pi$ state corresponds to a hole (holon-spinon bound state) plus a magnon (spinon-spinon bound state). The trial wave functions are given by $|\psi_{\rm trial}\rangle = \mathcal{N}(|\psi_{+}\rangle + \mathrm{a}|\psi_{-}\rangle)$, where $|\psi_{+}\rangle$ is the trial wave function constructed with the flux configuration shown in figure 3b and $|\psi_{-}\rangle$ its P or T conjugate. The boundary phase for the flux band structure before projection has been 0 for the chain containing the holon, and π for the other chain.

J_{\perp}	J_{\perp}/J		$E_{ m tot}$		over-	$E_{J_{\parallel}}$		$E_{J_{\perp}}$		a
	k_x/π				lap					
	0				0.844					
	1/4	-6.16	-6.13	0.4	0.994	-6.08	-6.08	-0.08	-0.05	0.01
0.2	1/2	-5.60	-5.56	0.7	0.983	-5.44	-5.47	-0.16	-0.09	0.04
	3/4	-5.96	-5.89	1.1	0.961	-5.70	-5.73	-0.26	-0.16	0.22
	1	-6.98	-6.94	0.6	0.990	-6.73	-6.76	-0.25	-0.18	1.00
	0	-7.33	-6.99	4.6	0.885	-5.11	-3.79	-2.22	-3.20	1.00
	1/4	-7.24	-7.01	3.1	0.927	-4.78	-3.74	-2.46	-3.27	0.43
1					0.961					
	3/4	-7.96	-7.87	1.1	0.981	-4.56	-4.22	-3.39	-3.65	0.10
	1	-8.73	-8.63	1.1	0.982	-5.68	-5.36	-3.04	-3.27	1.00
	0	-4.91	-4.86	1.0	0.986	-0.04	0.12	-4.88	-4.99	1.00
5	1/4				0.988					
	1/2	-5.09	-5.06	0.6	0.991	-0.18	-0.08	-4.91	-4.97	1.03
	3/4	-5.24	-5.20	0.7	0.991	-0.34	-0.23	-4.90	-4.98	1.03
	1	-5.31	-5.26	0.9	0.987	-0.43	-0.28	-4.88	-4.99	1.00

TABLE III. As in table II, but now for spinon-spinon bound states (magnons) with $k_y = \pi$ obtained by creation of an electron at the holon site. For $k_x = 0$, spinetto-spinon bound states yield better trial wave functions (the energy is only 0.4 % off at $J_{\perp}/J = 0.2$, and 2.7 % off at $J_{\perp}/J = 1$).

t/J	E_{tot}		%	over-	$E_{t_{\parallel}}$		$E_{t_{\perp}}$		a
	exact	trial	off	lap	exact	rial	exact	trial	
0	-8.18			0.888					1.00
		-8.00	2.2	0.938		0.00		0.00	*
0.2	-8.37			0.927					
		-8.12	2.9	0.923		0.00		-0.13	*
0.5	-8.87			0.929					
		-8.32	6.3	0.862		0.00		-0.32	*
1	-9.89	-9.52	3.7	0.894	-1.54	-1.23	-0.59	-0.57	0.02
2	-12.1	-11.3	6.5	0.797	-3.36	-2.63	-1.31	-1.02	0.04
5	-19.5	-16.8	14	0.585	-8.86	-6.84	-3.76	-2.33	0.08

TABLE IV. As in table II, but now with $J_{\perp}/J = t_{\perp}/t = 1$ for different ratios t/J. The momentum is $(k_x, k_y) = (\pi/2, 0)$, which corresponds to the ground state of the 2×8 ladder with periodic boundary conditions. For $t/J \leq 0.5$, data for holetto-spinon bound states are shown as well, marked with *; these adequately describe stationary holes (t = 0).

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